

Ethyl 4-ethoxybutyrate

26448-91-9 | DTXSID10403149

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.72	51.8	0.74	50.3	0.73	52.7

Model Results

Predicted value: -53.9 °C

Global applicability domain: Inside

Local applicability domain index: 7.66e-01

Confidence level: 6.26e-01

Nearest Neighbors from the Training Set

[Image not found](#)

2-Butoxyethyl acetate

Measured: -63.0

Predicted: -54.2

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2-Ethoxyethyl acetate

Measured: -61.7

Predicted: -56.7

[Image not found](#)

2-Ethoxyethyl acrylate

Measured: -47.0

Predicted: -54.7

[Image not found](#)

2-Methoxyethyl acetate

Measured: -70.0

Predicted: -63.1

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Dimethyl decanedioate

Measured: 38.0

Predicted: 1.98